Sub-gap in the Edge States of 2-D Chiral Superconductor with Rough Surface

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We discuss the rough surface effects on a two-dimensional chiral $k_x + ik_y$ superconductor. The atomic scale roughness at the surface is considered using the random S matrix model. The roughness effects on the self-consistent order parameter, the surface mass current and the surface density of states are studied using the quasi-classical theory. We find that the surface mass current is suppressed by the surface roughness. The surface density of states shows a quite similar behavior to that of superfluid ^{3}He B phase. When the surface is specular, the surface Andreev bound states form a band which fills the bulk energy gap $\Delta_{\rm bulk}$. When the surface becomes diffusive, there occurs a sharp upper edge of the surface bound states band and there opens a sub-gap between the edge and the bulk energy gap. We show that this sub-gap is induced by the repulsion between the surface bound states and the propagating Bogoliubov quasi-particles through the second order process of roughness.

KEYWORDS: 2-D Chiral Superconductor, Edge States, Surface Demsity of States, Superfluid ^{3}He-B

The 2-dimensional chiral $k_x + ik_y$ state is known as a model system for Sr_2RuO_4 superconducting state.[1] When there is a surface along the y axis, there occur gapless surface Andreev bound states as in other p-wave[2,3] and d-wave[4] pairing systems, because the k_x component of the order parameter changes its sign under the surface reflection. The surface bound states in chiral system are known to carry spontaneous mass flow along the surface.[5,6] Recently, surface bound states are recognized as edge states which reflect the topological nature of the bulk pairing state. A lot of attention has been paid to the surface Andreev bound states from this aspect.[6–15]

In this paper, we consider the effects of atomic scale surface roughness on the chiral k_x+ik_y state. We use the quasi-classical theory[16,17] developed for the study of p-wave Fermi superfluids. We calculate the self-consistent order parameter, the surface mass current and the surface density of states. The surface density of states shows quite a similar behavior to that in the 3-dimensional BW state.[17] Existence of the order parameter component parallel to the surface disperses the surface bound state energy. The bound states, therefore, form a band below the bulk energy gap $\Delta_{\rm bulk}$. When the surface is specular, the band completely fills the bulk energy gap. When the surface becomes diffusive, however, there occurs a sharp upper edge of the band and there opens a sub-gap between the edge and the bulk energy gap. The band edge energy Δ^* increases as the roughness is reduced. Similar sub-gap has been known in the BW state.[17–19] The sub-gap was first reported by Zhang[18] who treated the surface roughness using the thin dirty layer model. He suggested that the sub-gap is due to the suppression of the parallel component of the order parameter by the roughness. However, Nagato et al.[17] found that this sub-gap also occurs when the order parameter is assumed to be spatially constant. Although the existence of the sub-gap played a decisive role in the interpretation of the transverse acoustic impedance of the B phase of superfluid ^{3}He,[20–23] the origin of the sub-gap has been a puzzle for a long time.

We consider a two-dimensional k_x+ik_y superconductor which fills the $x > 0$ domain. The surface extends along the y axis. Since the order parameter is suppressed near the surface, the order parameter will take a form

$$\Delta(\hat{\boldsymbol{k}}, x) = \Delta_\perp(x)\hat{k}_x + i\Delta_\parallel(x)\hat{k}_y = \Delta_\perp(x)\cos\phi + i\Delta_\parallel(x)\sin\phi, \tag{1}$$

where ϕ is the angle between the Fermi momentum and the x axis.

We investigate the effects by surface roughness of atomic scale using random S-matrix model.[16,17,23] The surface is characterized by an S-matrix for the quasiparticles at the Fermi level in the normal state

$$S_{k_y,q_y} = -\left(\frac{1-i\eta}{1+i\eta}\right)_{k_y q_y}, \tag{2}$$

where $k_y(q_y)$ is the y component of the incident (scattered) Fermi momentum and η is a Hermite matrix that specifies the surface roughness. We assume that η is a random Hermite matrix which obeys $\overline{\eta_{k_y q_y}} = 0$ and $\overline{\eta^*_{k_y q_y}\eta_{k'_y q'_y}} = 2W/(\sum_{q_y} 1)\delta_{k_y-q_y,k'_y-q'_y}$ with W a parameter that specifies the roughness of the surface. One can show that $W = 1$ corresponds to the diffusive surface boundary condition and $W = 0$ corresponds to the specular surface boundary condition.[16,17]

Taking into account the surface roughness within the self-consistent Born approximation, we obtain the quasi-classical Green's function at the surface.[17,23]

$$G_\pm(k_y, 0) = G_S + (G_S \pm i)\frac{1}{G_S^{-1} - \Sigma}(G_S \mp i), \tag{3}$$

$$\Sigma = 2W\left\langle \frac{1}{G_S^{-1} - \Sigma} \right\rangle. \tag{4}$$

Here $G_+(k_y, 0)$ and $G_-(k_y, 0)$ are the quasi-classical Green's function for the Fermi momentum $(k_x > 0, k_y)$ and $(k_x < 0, k_y)$, respectively. G_S is the quasi-classical

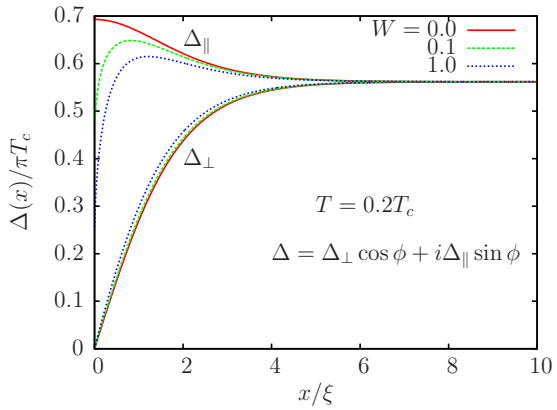

Fig. 1. (color online) Self-consistent order parameter of $k_x + ik_y$ state is plotted against the distance from the surface scaled by the coherence length $\xi = v_F/\pi T_c$ for some typical values of the roughness parameter W.

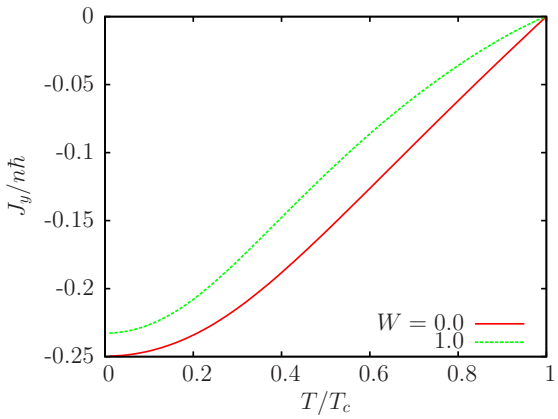

Fig. 2. (color online) Temperature dependence of the total current J_y along the y axis. Solid curve is for the specular surface ($W = 0$) and the dotted curve is for the diffusive surface ($W = 1$).

Green's function at $x = 0$ for the specular surface and Σ is the surface self energy which is induced by the roughness. The angle average in the two-dimensional system is

$$< \cdots > = \frac{\int dk_y \cdots}{\int dk_y 1} = \frac{1}{2}\int_{-\pi/2}^{\pi/2} d\phi \cos\phi \ \cdots . \quad (5)$$

The quasi-classical Green's function $G_\pm(k_y, x)$ at finite x is calculated by evolution operator technique.[16,17)]

Using the Matsubara Green's function, we can calculate the self-consistent order parameter and the edge mass current. In Fig. 1, we show the self-consistent order parameter at $T = 0.2T_c$. Since the bulk energy gap is isotropic in the two-dimensional $k_x + ik_y$ state, the order parameter shows a quite similar profile to that of the three-dimensional BW state. The perpendicular component $\Delta_\perp(x)$ is suppressed near the surface. In case of the specular surface,[5)] the parallel component $\Delta_\parallel(x)$ is enhanced near the surface such that compensates the loss of the condensation energy caused by the suppression of the perpendicular component $\Delta_\perp(x)$. In case of the diffusive surface, $\Delta_\parallel(x)$ is also suppressed by the incoherent phase mixing during the reflection processes.[24)]

Once the order parameter is determined, the surface mass current along the y axis can be calculated from the diagonal element of the quasi-classical Green's function. In Fig. 2, we show the total surface mass current J_y, current density integrated over x, as a function of temperature. In case of the specular surface ($W = 0$), the total current tends to $J_y = -n\hbar/4$ as $T \to 0$K.[6)] Here, n is the total number density. When the surface is diffusive ($W = 1$), the total current is definitely suppressed. The suppression of the mass current by surface roughness was discussed by Ashby and Kallin[24)] using GL theory.

The surface density of states can be calculated from the quasi-classical Green's function with real frequency ϵ. We show the angle resolved density of states in Fig. 3 for the diffusive surface ($W = 1$). In case of the specular surface, the surface density of states shows a delta function peak that corresponds to the surface Andreev bound state. The peak position is roughly equal to $\Delta_\parallel(0)\sin\phi$.

When integrated over the angle, therefore, the bulk energy gap below $\Delta_{\rm bulk}$ is filled by the bound states. In case of the diffusive surface, the bound state peak is broadened and is shifted towards the lower energy. Moreover, there appears a sharp upper energy edge Δ^* common to all the incident angles, which leads to a sub-gap between Δ^* and $\Delta_{\rm bulk}$.

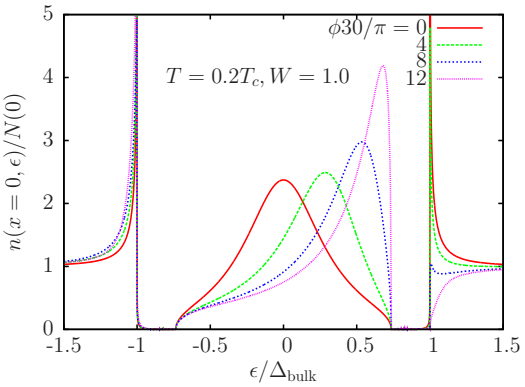

Fig. 3. (color online) Angle resolved surface density of states in case of the diffusive surface ($W = 1$). Incident angles are $\phi = 0, \frac{4}{30}\pi, \frac{8}{30}\pi$ and $\frac{12}{30}\pi$.

To examine the origin of the sub-gap, we consider Green's function at the surface given by Eqs. (3) and (4). To discuss the density of states below the bulk energy gap $\Delta_{\rm bulk}$, we consider real frequency $|\epsilon| < \Delta_{\rm bulk}$. Let us first consider G_S which is given by[17,23)]

$$G_S = \frac{1}{1-D^2}\begin{pmatrix} i(1+D^2) & -2D \\ -2D & -i(1+D^2) \end{pmatrix}, \quad (6)$$

where $D = D(0, \epsilon, k_y)$ is a solution at $x = 0$ of the Ricatti equation

$$v_F \cos\phi \frac{\partial}{\partial x} D = -2i\epsilon D + \Delta(\hat{k}, x)D^2 - \Delta^*(\hat{k}, x) \quad (7)$$

with the boundary condition at the bulk infinity

$$D(\infty,\epsilon,k_y)=\frac{i\Delta^*(\hat{k},\infty)}{\epsilon+\sqrt{\epsilon^2-|\Delta_{\rm bulk}|^2}}=e^{i(\alpha-\phi)}, \quad (8)$$

where we have defined $\alpha=\sin^{-1}(\epsilon/\Delta_{\rm bulk})$. For the energy $|\epsilon|<\Delta_{\rm bulk}$, it can be shown from Eq. (7) that $|D(x,\epsilon,k_y)|$ is always unity, therefore we may write

$$D(x,\epsilon,k_y)=e^{i\theta(x,\epsilon,k_y)} \quad (9)$$

with θ the real function. Solving Eq. (7) for a given k_y, we find an ϵ that satisfies

$$D(0,\epsilon,k_y)=1. \quad (10)$$

This energy is the surface bound state energy for the specular surface because the Green's function G_S has a pole at that energy. It is worth noting that D is related to the Nambu amplitude $(u(x),v(x))$ of the state with energy ϵ. The ratio of the hole component v to the particle component u is given by $v/u=(-i)D$. It follows that the hole-particle ratio v/u at the surface is equal to $-i$ for all the surface bound states.

When we assume that the order parameters are constant, i.e., $\Delta_\perp(x)=\Delta_\parallel(x)=\Delta_{\rm bulk}$, D is also a constant given by Eq. (8). The bound states have a linear dispersion relation $\epsilon=\Delta_{\rm bulk}\sin\phi=\Delta_{\rm bulk}\hat{k}_y$ and can be regarded as Majorana-Weyl Fermions.[6)]

Now we consider the surface self energy. From Eqs. (4) and (6), we may parametrize the self energy in a form

$$\Sigma=\begin{pmatrix} is_3 & s_1 \\ s_1 & -is_3\end{pmatrix}. \quad (11)$$

It is convenient to introduce projection operators $P_\pm=\frac{1}{2}(1\pm\rho_2)$ with ρ_2 a Pauli matrix in particle-hole space. Then we can write

$$\Sigma=i\rho_3\left(P_+(s_3+s_1)+P_-(s_3-s_1)\right), \quad (12)$$

$$G_s=i\rho_3\left(P_+\frac{1-D}{1+D}+P_-\frac{1+D}{1-D}\right). \quad (13)$$

It is obvious from Eq. (13) that P_+ projects out the surface bound states. From Eqs. (4), (12) and (13), we find that

$$s_3+s_1=2W\left\langle\frac{1-D}{(1+(s_3-s_1))+(1-(s_3-s_1))D}\right\rangle, \quad (14)$$

$$s_3-s_1=2W\left\langle\frac{1+D}{(1+(s_3+s_1))-(1-(s_3+s_1))D}\right\rangle. \quad (15)$$

The density of states is given by the imaginary part of the diagonal element of the quasi-classical Green's function given by Eqs. (3), (12) and (13).[17)]

$$\begin{aligned}G_+^{11}=&G_-^{11}\\ =&\frac{i}{2}\left(\frac{(1+(s_3+s_1))+(1-(s_3+s_1))D}{(1+(s_3+s_1))-(1-(s_3+s_1))D}\right.\\ &\left.+\frac{(1+(s_3-s_1))-(1-(s_3-s_1))D}{(1+(s_3-s_1))+(1-(s_3-s_1))D}\right). \quad (16)\end{aligned}$$

When the energy is in the range $|\epsilon|<\Delta_{\rm bulk}$, D is given from Eq. (9) by a form $e^{i\theta(0,\epsilon,k_y)}$. It follows that if both s_3 and s_1 are pure imaginary, the diagonal element of the Green's function is real, namely there is no density of states. At the sub-gap energies, therefore, s_3, s_1 are expected to take pure imaginary values. At first sight, both Eqs. (14) and (15) have pure imaginary solutions. Both the equations are invariant under the complex conjugate transformation because $D=e^{i\theta}$. The real part emerges when there appears a pole along the angle integral in Eqs. (14) and (15).

From now on, for simplicity, we consider a case where the order parameters are constant and the roughness parameter W is small. When the order parameter is constant, $D=e^{i(\alpha-\phi)}$; therefore, the bound state energy for the specular surface is given from $D=1$ by $\alpha=\phi$ ($\epsilon=\Delta_{\rm bulk}\sin\phi$). Within the lowest order correction with respect to W, s_3+s_1 remains pure imaginary because the bound states are projected out in Eq. (14).

$$s_3+s_1=2W\langle(-i){\rm Tr}(P_+\rho_3G_s)\rangle=2W\left\langle\frac{1-D}{1+D}\right\rangle \quad (17)$$

$$=iW\left(\cos\alpha\ln\left|\frac{1+\sin\alpha}{1-\sin\alpha}\right|-\pi\sin\alpha\right)\equiv\frac{i}{2}f(\alpha). \quad (18)$$

On the other hand, s_3-s_1 acquires real part because Eq. (15) has a pole of the surface bound state when s_3+s_1 is neglected. Let us consider the next order correction by W to the possible pole of Eq. (15)

$$D=\frac{1+(s_3+s_1)}{1-(s_3+s_1)}. \quad (19)$$

When W is small, the possible pole will occur near $D\sim 1+i(\alpha-\phi)$. Expanding both sides of Eq. (19) in terms of small quantities, we obtain

$$\alpha-\phi=(-2i)(s_3+s_1)=f(\alpha). \quad (20)$$

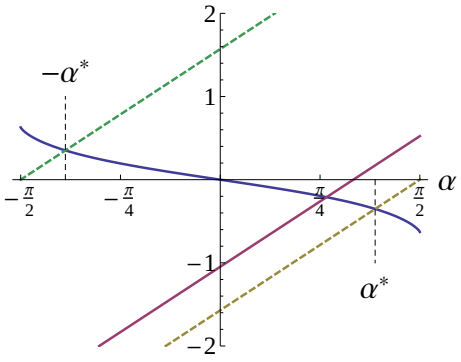

Fig. 4. (color online) $\alpha-\phi$ ($\phi=-\pi/2,\pi/3,\pi/2$) and $f(\alpha)$ with $W=0.1$ are plotted.

We plot the both hand sides of Eq. (20) in Fig. 4 as functions of $\alpha=\sin^{-1}(\epsilon/\Delta_{\rm bulk})$. Since $f(\alpha)$ is a decreasing odd function of α, there is a solution of Eq. (20) for any $-\pi/2<\phi<\pi/2$. But, when we define α^* at which

the straight line $\alpha - \pi/2$ and $f(\alpha)$ crosses;

$$\alpha^* - \pi/2 = f(\alpha^*), \tag{21}$$

we find that there is no solution of Eq. (20) for α in the range $\alpha^* < |\alpha| < \pi/2$. It means that Eq.(15) has no pole and $s_3 - s_1$ remains pure imaginary in that energy range. As a result, for all the incident angles there occurs a common sub-gap in the energy range $\Delta^* = \Delta_{\rm bulk} \sin\alpha^* < |\epsilon| < \Delta_{\rm bulk}$, as seen in Fig. 3. Solving Eq. (21) with respect to α^*, we obtain $\Delta^* = \Delta_{\rm bulk} \sin\alpha^*$ as a function of W. The result is plotted in Fig. 5 together with the self-consistent solution of Eq. (4).

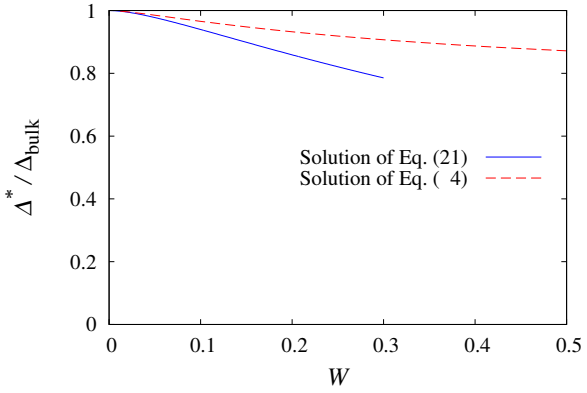

Fig. 5. (color online) Δ^* vs W. Order parameters are assumed to be spatially constant. Dashed curve is a result of self-consistent solution of Eq. (4). Solid curve is a result of Eq. (21).

The origin of the sub-gap is interpreted in a following way. Since Eq. (19) is also a possible pole of the diagonal element $G^{11}_{\pm}$ of the Green's function (see Eq. (16)), Eq. (20) is interpreted to be an equation to determine the energy of the bound state with finite W, although we have used it to find out the energy range without solution. Equation (20) with (17) has a similar form to the denominator of the usual Green's function for the impurity problem within the Born approximation, therefore it corresponds to the Brillouin-Wigner perturbation formula

$$\epsilon - \epsilon_n^{(0)} = \sum_m \frac{|V_{nm}|^2}{\epsilon - \epsilon_m^{(0)}}, \tag{22}$$

where $\epsilon_n^{(0)}$ corresponds to $\Delta_{\rm bulk} \sin\phi$ and $|V_{nm}|^2$ to W. Since the bound states are projected out in Eqs. (17) and (20), the intermediate states are the propagating Bogoliubov quasi-particle states with energy $|\epsilon| > \Delta_{\rm bulk}$. The right hand side of Eq. (22) becomes a decreasing odd function of ϵ and reproduces the α dependence of $f(\alpha)$. The sub-gap comes out, thus, as a result of the repulsion between the bound state and the propagating states through the second order process. This scenario does not change in case of the self-consistent order parameter, although Eq. (20) should be calculated numerically. The sub-gap in superfluid ^{3}He-B can be explained in a similar manner.

It is of interest if the sub-gap which has been observed in the B phase of superfluid ^{3}He can be also observed in Sr_2RuO_4, for example by tunneling experiment.[25,26] For comparison with experiment, the effects by finite transmittance of the rough interface should be examined.[27] Such a study shall be reported elsewhere.

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1) A. P. Mackenzie and Y. Maeno: Rev. Mod. Phys. **75**(2003) 657.
2) L. J. Buchholtz and G. Zwicknagl: Phys. Rev. B **23** (1981) 5788.
3) J. Hara and K. Nagai: Prog. Theor. Phys. **76** (1986) 1237.
4) C. R. Hu: Phys. Rev. Lett. **72** (1994) 1526.
5) M. Matsumoto and M. Sigrist: J. Phys. Soc. Jpn. **68** (1999) 994.
6) M. Stone and R. Roy: Phys. Rev. B **69** (2004) 184511.
7) G. E. Volovik: JETP Lett. **66** (1997) 522.
8) A. P. Schnyder, S. Ryu, A. Furusaki and A. W. W. Ludwig: Phys. Rev. B **78** (2008) 195125.
9) R. Roy: arXiv:0803.2868v1 (2008)
10) A. Kitaev: AIP Conf. Proc. **1134** (2009) 22.
11) X.-L. Qi, T.L. Hughes, S. Raghu and S.-C.Zhang: Phys. Rev. Lett. **102** (2009) 187001.
12) S. B. Chung and S.-C. Zhang: Phys. Rev. Lett. **103** (2009) 235301.
13) G. E. Volovik: Pis'ma Zh. Eksp. Teor. Fiz. **90** (2009) 440.
14) Y. Nagato, S. Higashitani and K. Nagai: J. Phys. Soc. Jpn. **78** (2009) 123603.
15) S. Murakawa, Y. Wada, Y. Tamura, M. Wasai, M. Saitoh, Y. Aoki, R. Nomura, Y. Okuda, Y. Nagato, M. Yamamoto, S. Higashitani and K. Nagai: J. Phys. Soc. Jpn. **80** (2011) 013602.
16) Y. Nagato, S. Higashitani, K. Yamada and K. Nagai: J. Low Temp. Phys. **103** (1996) 1.
17) Y. Nagato, M. Yamamoto and K. Nagai: J. Low Temp. Phys. **110** (1998) 1135.
18) W. Zhang: Phys. Lett. A **130** (1988) 314.
19) A. B. Volontsov and J. A. Sauls: Phys. Rev. B. **68** (2003) 064508.
20) Y. Aoki, Y. Wada, N. Saitoh, R. Nomura, Y. Okuda, Y. Nagato, M. Yamamoto, S. Higashitani and K. Nagai: Phys. Rev. Lett. **95** (2005) 075301.
21) S. Murakawa, Y. Tamura, Y. Wada, M. Wasai, M. Saitoh, Y. Aoki, R. Nomura, Y. Okuda, Y. Nagato, M. Yamamoto, S. Higashitani and K. Nagai: Phys. Rev. Lett. **103** (2009) 155301.
22) Y. Nagato, M. Yamamoto, S. Higashitani and K. Nagai: J. Low Temp. Phys. **149** (2007) 294.
23) K. Nagai, Y. Nagato, M. Yamamoto and S. Higashitani: J. Phys. Soc. Jpn. **77** (2008) 111003.
24) P. E. C. Ashby and C. Kallin: Phys. Rev. B **79** (2009) 224509 .
25) F. Laube, G. Goll, H. v. Löhneysen, M. Fogelström and F. Lichtenberg: Phys. Rev. Lett. **84** (2000) 1595.
26) S. Kashiwaya, H. Kashiwaya, H. Kambara, T. Furuta, H. Yaguchi, Y. Tanaka and Y. Maeno: Phys. Rev. Lett. **107** (2011) 077003.
27) Y. Nagato amd K. Nagai: Phys. Rev. B **69** (2004) 104507.